

Effects of disorder on the vortex charge

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We study the influence of disorder on the vortex charge, both due to random pinning of the vortices and due to scattering off non-magnetic impurities. In the case when there are no impurities present, but the vortices are randomly distributed, the effect is very small, except when two or more vortices are close by. When impurities are present, they have a noticeable effect on the vortex charge. This, together with the effect of temperature, changes appreciably the vortex charge. In the case of an attractive impurity potential the sign of the charge naturally changes.

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I. INTRODUCTION

Some time ago¹ it was proposed that the vortex induced by an external magnetic field in a type-II superconductor should be electrically charged. This effect was proposed to occur since the chemical potential is expected to be larger in the vortex core than in the bulk of the superconductor. It is energetically favorable for the electrons to lower their energy through the condensation energy and, since the vortex core is interpreted as being a normal region, the electrons tend to move to the bulk leaving a charge deficiency close to the vortex line. It is the electrochemical potential (the sum of the chemical potential and electrostatic energy) that is constant in the superconductor. Due to the circulating currents around the vortex line the electrostatic potential is needed to compensate the centrifugal force due to the circular motion².

We should note that the initial understanding that the vortex core region is populated by normal electrons has been questioned. In particular, in the case of clean superconductors, where the mean free path is much larger than the coherence length, the localized states bound to the vortex core are the result of Andreev scattering³. The core states are coherent superpositions of particle and hole states and interpreted as being the result of constructive interference of multiple Andreev scattering from the spatial variation of the order parameter. Also it was shown that the main contribution to the supercurrent is originated in these states.

Soon after the proposal of Khomskii and Freimuth it was suggested that the effect could be tested experimentally due to the dipole field created at the surface of the superconductor⁴. It has been claimed that the charge of the vortex has been measured using NMR in high temperature superconductors⁵.

Theoretical studies on the existence of the vortex charge were carried out subsequently^{6,7,8,9}. In particular, a relation was established between the vortex core

charge and the vortex bound states for an s-wave vortex⁶. In particular, in the quantum limit the influence of the bound states is important. This regime is reached when $T/T_c \leq 1/(k_F \zeta_0)$, where T_c is the critical temperature, k_F is the Fermi momentum and $\zeta_0 = v_F/\Delta_0$ is the coherence length, corresponding to a regime where the thermal width is smaller than the level spacing. In this regime the particle-hole asymmetry in the local density of states (LDOS) has been related to the vortex charge⁶. The asymmetry results from the different effect the supercurrent around the vortex has on the particle and hole wave functions¹⁰. However, in d-wave superconductors the low lying states are not localized¹¹. As shown recently, it is the winding of the phase around the vortex and not the detailed decreasing of the gap amplitude near the vortex core that is ultimately responsible for the supercurrent and the nature of the low-lying states (bound states in the s-wave case) and their effect on many properties^{10,12}, such as the vortex charge.

Taking into account the screening of the vortex charge, the Friedel oscillation in the charge profile was obtained for the case of a s-wave vortex⁷, showing that the charge is screened but prevails with a somewhat reduced value. Other pairing symmetries were also considered^{8,13} showing that the existence of the vortex charge is universal. In all these studies the vortex is charged positively (electron deficiency). This positive charge has been argued to be the cause of the Hall anomaly where the Hall conductance changes sign when entering the superconducting phase¹⁴.

In the high magnetic field regime, where a Landau level description is appropriate, the low lying states are coherent through the vortex lattice¹⁵ both in the s-wave¹⁵ and in the d-wave cases¹⁶. The coherent nature of the states originates gapless superconductivity due to the center of mass motion of the Cooper pairs and the action of a high magnetic field^{15,17}. In this regime the vortex charge has not yet been studied.

In d-wave superconductors it is likely that other order-

ings compete with the superconductivity. In particular, antiferromagnetism¹⁸, or d-density waves¹⁹. The vortex structure and, in particular, the vortex charge, have also been studied when there is competition between the various order parameters^{13,20,21,22,23}. In general, a small region around the vortex will have a non-vanishing order parameter which affects the density of states and in particular the vortex charge. It may change sign from an electron deficiency to an electron abundance at the vortex core. Also, increasing the temperature, in a regime of parameters where the competing order is absent, the positive vortex charge is recovered²¹.

Also, since most systems have impurities, these affect both the motion of the quasiparticles through scattering and through pinning of the vortices. Therefore it is necessary to study the effect of the impurities. Such a study has been carried out in the case of the d-density wave state²⁴. It is clear that, at the very least, the effect of the addition of the impurities is to locally change the chemical potential.

In this work we consider several causes for disorder and their effect on the vortex charge. The effect of a charge inside a superconductor is in general screened. In usual superconductors of the *s*-wave type, the dominant contribution is due to Thomas-Fermi like screening, as in the normal state²⁵. Due to the presence of the gap the Fermi surface Friedel oscillations are suppressed. The exponential screening acts on the scale of the Thomas-Fermi length which in general is much smaller than the coherence length, and therefore any charge is very small. However, in *d*-wave superconductors or in *s*-wave superconductors in the vicinity of a vortex, the Friedel oscillations are important since in the first case there are gapless states and in the second case there are states of an essentially normal character in the vicinity of the vortex core⁷. These oscillations act on a scale which is comparable to the coherence length, which in type-II superconductors is small. Therefore in the vicinity of the vortex core the screening effect, even though noticeable, does not change qualitatively the effect of the charge depletion. This is shown in Fig. 1 of ref.⁷ where the charge oscillations near the core, even though depressed, are still visible and only a quantitative change is observed. Therefore, for simplicity, we will neglect in this work the effect of screening since the results will be qualitatively the same. Also, as we will show later, the effect of the impurities has a local nature and only affects significantly the physical quantities near the vortex core where screening has not fully acted. Only far from the vortex core the screening of the Thomas-Fermi type will strongly suppress the charge oscillations⁷.

II. VORTICES AT LOW TO INTERMEDIATE FIELDS

Consider the lattice formulation of a superconductor in a magnetic field. Let us start from the Bogoliubov-de

Gennes equations $\mathcal{H}\psi = \epsilon\psi$ where $\psi^\dagger(\mathbf{r}) = (u^*(\mathbf{r}), v^*(\mathbf{r}))$ and where the matrix Hamiltonian is given by

$$\mathcal{H} = \begin{pmatrix} \hat{h} & \hat{\Delta} \\ \hat{\Delta}^\dagger & -\hat{h}^\dagger \end{pmatrix} \quad (1)$$

with^{26,27}

$$\hat{h} = -t \sum_{\delta} e^{-\frac{i\epsilon}{\hbar c} \int_{\mathbf{r}}^{\mathbf{r}+\delta} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{l}} \hat{s}_{\delta} - \epsilon_F \quad (2)$$

and

$$\hat{\Delta} = \Delta_0 \sum_{\delta} e^{\frac{i}{2}\phi(\mathbf{r})} \hat{\eta}_{\delta} e^{\frac{i}{2}\phi(\mathbf{r})}. \quad (3)$$

The sums are over nearest neighbors ($\delta = \pm\mathbf{x}, \pm\mathbf{y}$ on the square lattice); $\mathbf{A}(\mathbf{r})$ is the vector potential associated with the uniform external magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, the operator \hat{s}_{δ} is defined through its action on space dependent functions, $\hat{s}_{\delta}u(\mathbf{r}) = u(\mathbf{r}+\delta)$, and the operator $\hat{\eta}_{\delta}$ describes the symmetry of the order parameter. It is convenient to perform a singular gauge transformation to eliminate the phase of the off-diagonal term (3) in the matrix Hamiltonian. We consider the unitary FT gauge transformation $\mathcal{H} \rightarrow \mathcal{U}^{-1}\mathcal{H}\mathcal{U}$, where²⁶

$$\mathcal{U} = \begin{pmatrix} e^{i\phi_A(\mathbf{r})} & 0 \\ 0 & e^{-i\phi_B(\mathbf{r})} \end{pmatrix} \quad (4)$$

with $\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = \phi(\mathbf{r})$. The phase field $\phi(\mathbf{r})$ is decomposed at each site of the two-dimensional lattice in two components $\phi_A(\mathbf{r})$ and $\phi_B(\mathbf{r})$ which are assigned respectively to a set of vortices *A*, positioned at $\{\mathbf{r}_i^A\}_{i=1,N_A}$, and a set of vortices *B*, positioned at $\{\mathbf{r}_i^B\}_{i=1,N_B}$. The phase fields $\phi_{\mu=A,B}$ are defined through the equation

$$\nabla \times \nabla \phi_{\mu}(\mathbf{r}) = 2\pi\mathbf{z} \sum_i \delta(\mathbf{r} - \mathbf{r}_i^{\mu}) \quad (5)$$

where the sum runs only over the μ -type vortices. After carrying out the gauge transformation (4) the Hamiltonian (1) reads

$$\mathcal{H}' = \begin{pmatrix} -t \sum_{\delta} e^{i\mathcal{V}_{\delta}^A(\mathbf{r})} \hat{s}_{\delta} - \epsilon_F & \Delta_0 \sum_{\delta} e^{-i\frac{\delta\phi}{2}} \hat{\eta}_{\delta} e^{i\frac{\delta\phi}{2}} \\ \Delta_0 \sum_{\delta} e^{-i\frac{\delta\phi}{2}} \hat{\eta}_{\delta}^\dagger e^{i\frac{\delta\phi}{2}} & t \sum_{\delta} e^{-i\mathcal{V}_{\delta}^B(\mathbf{r})} \hat{s}_{\delta} + \epsilon_F \end{pmatrix}. \quad (6)$$

The phase factors are given by²⁷ $\mathcal{V}_{\delta}^{\mu}(\mathbf{r}) = \int_{\mathbf{r}}^{\mathbf{r}+\delta} \mathbf{k}_s^{\mu} \cdot d\mathbf{l}$ and $\delta\phi(\mathbf{r}) = \phi_A(\mathbf{r}) - \phi_B(\mathbf{r})$, where $\hbar\mathbf{k}_s^{\mu} = m\mathbf{v}_s^{\mu} = \hbar\nabla\phi_{\mu} - \frac{\epsilon}{c}\mathbf{A}$ is the superfluid momentum vector for the μ -supercurrent. Physically, the vortices *A* are only visible to the particles and the vortices *B* are only visible to the holes. Each resulting μ -subsystem is then in an effective magnetic field

$$\mathbf{B}_{\text{eff}}^{\mu} = -\frac{mc}{e} \nabla \times \mathbf{v}_s^{\mu} = \mathbf{B} - \phi_0 \mathbf{z} \sum_i \delta^2(\mathbf{r} - \mathbf{r}_i^{\mu}) \quad (7)$$

where each vortex carries an effective quantum magnetic flux ϕ_0 . For the case of a regular vortex lattice^{26,27}, these effective magnetic fields vanish simultaneously on average if the magnetic unit cell contains two vortices, one of each type. More generally, in the absence of spatial symmetries, as it is the case for disordered systems, these effective magnetic fields $\mathbf{B}_{\text{eff}}^{\mu=A,B}$ vanish if the numbers of vortices of the two types A and B are equal, i.e. $N_A = N_B$, and their sum equals the number of elementary quantum fluxes of the external magnetic field penetrating the system.

The μ -superfluid wave vector $\mathbf{k}_s^\mu(\mathbf{r})$ characterizes the supercurrents induced by the μ -vortices. This vector can be calculated for an arbitrary configuration of vortices²⁷ like

$$\mathbf{k}_s^\mu(\mathbf{r}) = 2\pi \int \frac{d^2k}{(2\pi)^2} \frac{i\mathbf{k} \times \mathbf{z}}{k^2 + \lambda^{-2}} \sum_{i=1}^{\infty} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_i^\mu)}. \quad (8)$$

As we take the London limit, which is valid for low magnetic field and over most of the $H - T$ phase diagram in extreme type-II superconductors such as cuprates, we assume that the size of the vortex core is negligible and place each vortex core at the center of a plaquette.

For the conventional s -wave case the operator characterizing the symmetry of the order parameter is constant $\hat{\eta}_\delta = \frac{1}{4}$ and the off-diagonal terms of the Hamiltonian (6) are then considerably simplified

$$\mathcal{H}' = \begin{pmatrix} -t \sum_{\delta} e^{i\mathcal{V}_\delta^A(\mathbf{r})} \hat{s}_\delta - \epsilon_F & \Delta_0 \\ \Delta_0 & t \sum_{\delta} e^{-i\mathcal{V}_\delta^B(\mathbf{r})} \hat{s}_\delta + \epsilon_F \end{pmatrix}. \quad (9)$$

Note that in this case the phase of the off-diagonal term is eliminated.

For the unconventional d -wave case the operator $\hat{\eta}_\delta$ takes the form $\hat{\eta}_\delta = (-1)^{\delta_y} \hat{s}_\delta$. With these definitions the d -wave Hamiltonian can be derived from the Hamiltonian (6) and reads

$$\mathcal{H}' = \begin{pmatrix} -t \sum_{\delta} e^{i\mathcal{V}_\delta^A(\mathbf{r})} \hat{s}_\delta - \epsilon_F & \Delta_0 \sum_{\delta} e^{i\mathcal{A}_\delta(\mathbf{r}) + i\pi\delta_y} \hat{s}_\delta \\ \Delta_0 \sum_{\delta} e^{-i\mathcal{A}_\delta(\mathbf{r}) - i\pi\delta_y} \hat{s}_\delta & t \sum_{\delta} e^{-i\mathcal{V}_\delta^B(\mathbf{r})} \hat{s}_\delta + \epsilon_F \end{pmatrix} \quad (10)$$

where the phase factor $\mathcal{A}_\delta(\mathbf{r})$ has the form

$$\begin{aligned} \mathcal{A}_\delta(\mathbf{r}) &= \frac{1}{2} \int_{\mathbf{r}}^{\mathbf{r}+\delta} (\nabla\phi_A - \nabla\phi_B) \cdot d\mathbf{l} \\ &= \frac{1}{2} \int_{\mathbf{r}}^{\mathbf{r}+\delta} (\mathbf{k}_s^A - \mathbf{k}_s^B) \cdot d\mathbf{l}. \end{aligned} \quad (11)$$

In the Hamiltonian (10) and in Eq. 11 the vector

$$\mathbf{a}_s = \frac{1}{2} (\mathbf{k}_s^A - \mathbf{k}_s^B) \quad (12)$$

acts as an internal gauge field independent of the external magnetic field²⁷. The associated internal magnetic field

$\mathbf{b} = \nabla \times \mathbf{a}_s$ consists of opposite $A-B$ spikes fluxes carrying each one half of the magnetic quantum flux ϕ_0 , centered in the vortex cores and vanishing on average since the numbers of A - and B -type vortices are the same.

The solution of the BdG equations gives the spectrum and the wave functions of the quasiparticles. As the effective magnetic fields experienced by the particles and the holes vanish on average, within the gauge transformation we are allowed to use periodic boundary conditions on the square lattice ($\Psi(x+nL, y+mL) = \Psi(x, y)$ with $n, m \in \mathbb{Z}$). The $L \times L$ original lattice becomes then a magnetic supercell where the impurities are placed at random and where the vortices are placed in such a way as to minimize their total energy. The disorder induced by the impurities in the system is then established over a length L . Thus in order to compute the eigenvalues and eigenvectors of the Hamiltonian we seek for eigen-solutions in the Bloch form $\Psi_{n\mathbf{k}}^\dagger(\mathbf{r}) = e^{-i\mathbf{k} \cdot \mathbf{r}} (U_{n\mathbf{k}}^*, V_{n\mathbf{k}}^*)$ where \mathbf{k} is a point of the Brillouin zone. We diagonalize then the Hamiltonian $e^{-i\mathbf{k} \cdot \mathbf{r}} \mathcal{H} e^{i\mathbf{k} \cdot \mathbf{r}}$ for a large number of points \mathbf{k} in the Brillouin zone and for many different realizations (around 100) of the random impurity positions and of the correlated vortex positions.

The density of states (DOS) and the local density of states (LDOS) for the cases of vortex disorder³¹ and the combined effects of vortex disorder and impurity scattering³² were studied recently. The disorder in general increases the DOS at low energies, by filling the gap in the s -wave case and originating a finite density of states at zero energy in the d -wave case. An approximate scaling regime was obtained in the last case. Also, the results for the LDOS are in qualitative agreement with STM experiments if most vortices are pinned at the impurity locations.

The electron density is calculated in the usual way

$$n(\vec{r}) = 2 \sum_i (|u_i(\vec{r})|^2 f(E_i) + |v_i(\vec{r})|^2 (1 - f(E_i))) \quad (13)$$

where E_i are the energy eigenvalues and $f(E_i)$ is the Fermi function.

A. Vortex lattice

We consider first, for completeness, a regular distribution of vortices both for s -wave and d -wave pairings. At not very high fields, the vortices are sufficiently apart and the vortex charge is depleted from the vortex cores, as mentioned above. Therefore the vortices are positively charged. In Fig. 1 we consider the s -wave pairing case and in Fig. 2 we consider the d -wave pairing case. In this last case a checkerboard modulation of the charge density is seen. Both sets of results are presented for the case $\Delta = t$. Linearizing the BdG equations defined in a continuum close to the nodes leads naturally to the definition of two velocities the Fermi velocity, v_F , and a velocity $v_\Delta = \Delta_0/p_F$, where p_F is the Fermi momentum. This velocity denotes the slope of the gap at the

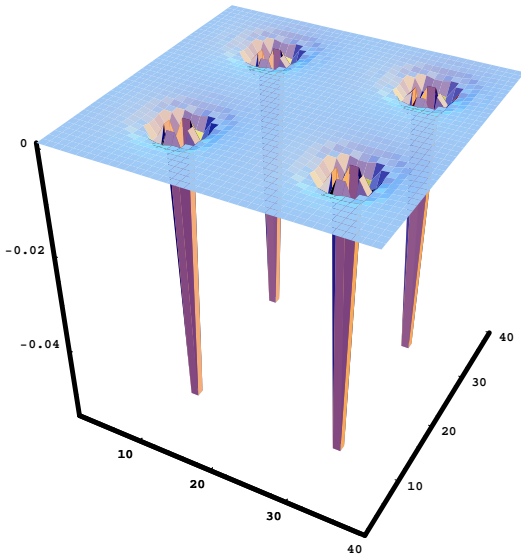


FIG. 1: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for s-wave symmetry in a regular vortex lattice. Here $\Delta = t$, $\mu = -2.2t$ and $n_{\text{bulk}} = 0.377$.

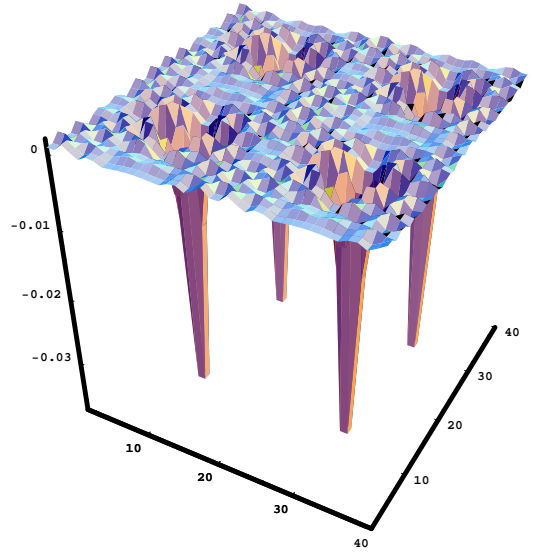


FIG. 3: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry in a regular vortex lattice. Here $\Delta = 0.25t$, $\mu = -2.2t$ and $n_{\text{bulk}} = 0.36$.

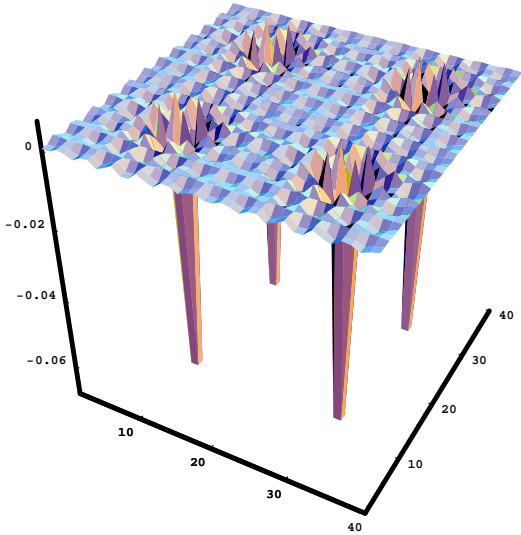


FIG. 2: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry in a regular vortex lattice. Here $\Delta = t$, $\mu = -2.2t$ and $n_{\text{bulk}} = 0.509$.

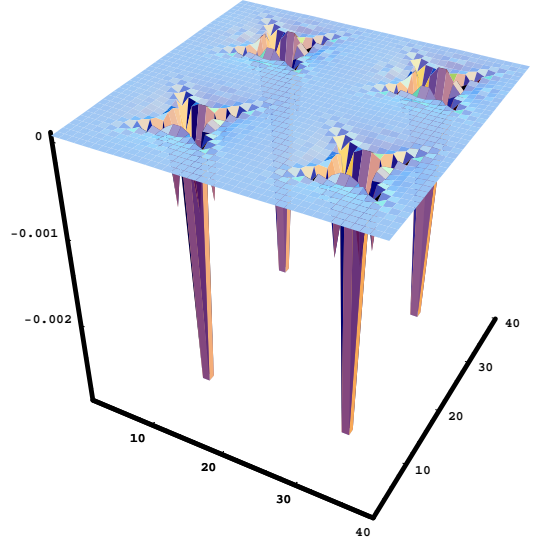


FIG. 4: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for s-wave symmetry in a regular vortex lattice. Here $\Delta = t$, $\mu = -0.1t$ and $n_{\text{bulk}} = 0.965$.

node^{26,33}. Defining the anisotropy of the Dirac cone as the ratio $\alpha_D = v_F/v_\Delta$ which in the lattice case translates to $\alpha_D = t/\Delta_0$, the case considered above $\Delta = t$ is called the isotropic case. In many d-wave superconductors the anisotropy is actually stronger. We present for comparison in Fig. 3 results for d-wave pairing considering $\Delta = 0.25t$ (note that in high- T_c materials the anisotropy is actually stronger of the order of $t = 15\Delta$). As the anisotropy increases the charge depletion decreases in depth but extends in area.

We have considered a low density regime. We can vary the chemical potential (and the band-filling). In Fig. 4 we present the electron density for a situation close to half-filling for the s-wave case. In Fig. 5 we consider a case larger than half-filling. In this case there is a charge accumulation (or hole depletion). Indeed as explained before⁶ the density of the dominant carriers is depleted near the vortex core. Also, we have checked explicitly that at half-filling the vortex charge vanishes⁶ and the electron density is uniform. The results for the d-wave

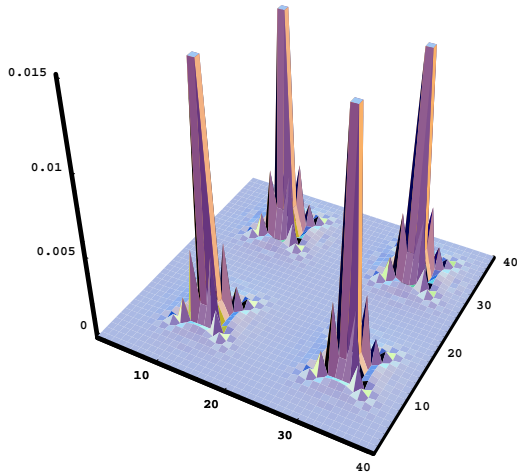


FIG. 5: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for s-wave symmetry in a regular vortex lattice. Here $\Delta = t$, $\mu = 0.5t$ and $n_{\text{bulk}} = 1.17$.

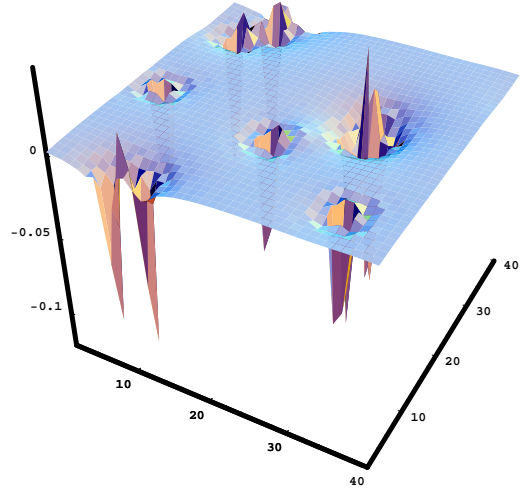


FIG. 6: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for s-wave symmetry in a disordered vortex lattice. Here the magnetic field is $B = 1/160$ which corresponds to 10 vortices in a 40×40 unit cell. Here $\Delta = t$, $\mu = -2.2t$ and $n_{\text{bulk}} = 0.375$.

case show the same trend.

B. Vortex disorder

We consider now the case when the vortices are distributed randomly due to some strong pinning effects, but neglect the effect of impurities on the motion of the quasiparticles. Therefore, the superfluid velocities are determined by a random distribution of the locations of the vortices, assumed static.

In Fig. 6 we consider the case of s-wave pairing and in Fig. 7 we consider d-wave pairing for a particular random distribution of the vortices (note that there is no sum over random configurations, like in the calculation of the LDOS). When a vortex is isolated the distortion of the charge profile is very similar to the lattice case. However, if two vortices are pinned nearby, the charge profile is significantly changed. In conjunction with the charge depletion, there is a sign reversal of the electron density. This is particularly visible in the s-wave case but also occurs for the d-wave symmetry. In the region where the two vortex cores are located there is a charge accumulation which leads to a local negative charge with respect to the bulk value. These fluctuations are of a similar order of magnitude as the charge depletion at the single vortices. However, the integration of the charge density in the neighborhood of the two vortices is still positive, despite the strong negative oscillations. The total charge in the case when two vortices are close by, even though still positive, is considerably smaller.

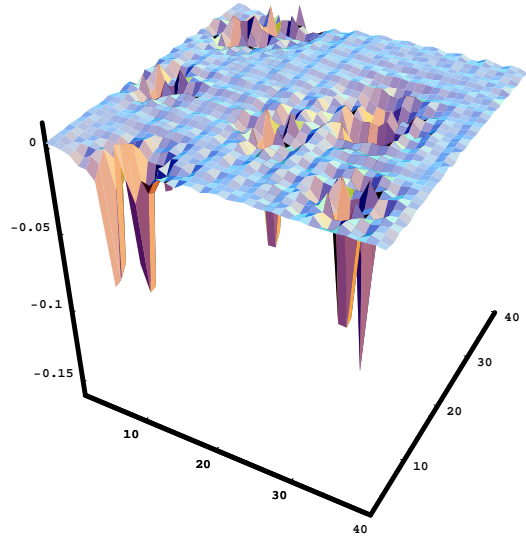


FIG. 7: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry in a disordered vortex lattice. Here the magnetic field is $B = 1/160$ which corresponds to 10 vortices in a 40×40 unit cell. Here $\Delta = t$, $\mu = -2.2t$ and $n_{\text{bulk}} = 0.507$.

C. Effect of impurities

We consider now the effect of impurities. These are introduced at the Hamiltonian level, with the substitution

$$\hat{h} \rightarrow \hat{h} + \mathcal{U}(\mathbf{r})$$

Here $\mathcal{U}(\mathbf{r})$ is the potential due to the impurities placed randomly in the system. We model the disorder using

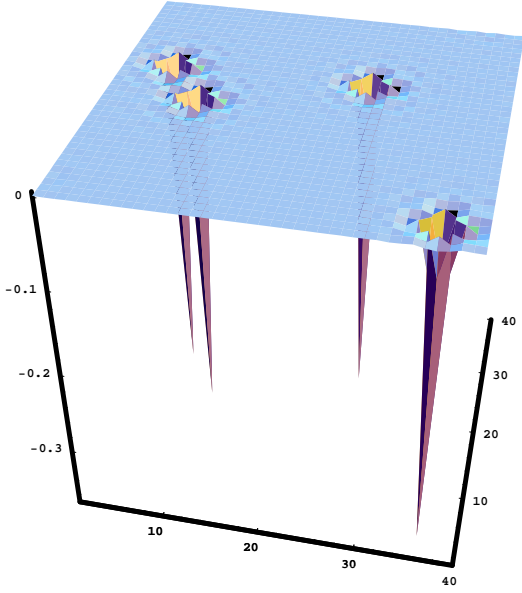


FIG. 8: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry with impurities and no vortices. Here $\Delta = t$, $\mu = -2.2t$, $U = 5t$ and $n_{\text{bulk}} = 0.509$.

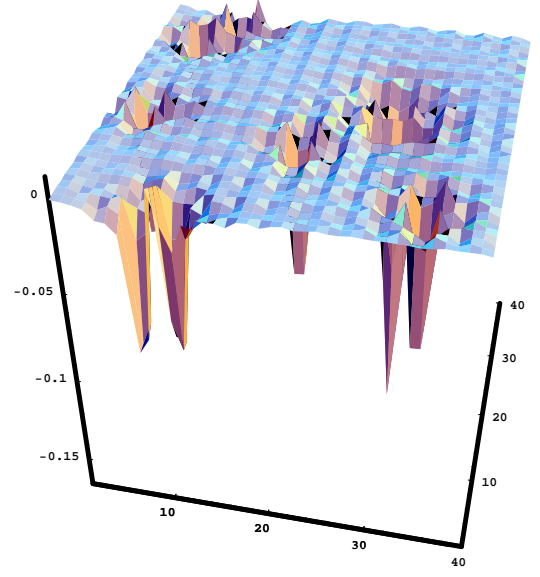


FIG. 10: (color online) Difference in the electron density between the cases with and without vortices shown in Figs. 8 and 9.

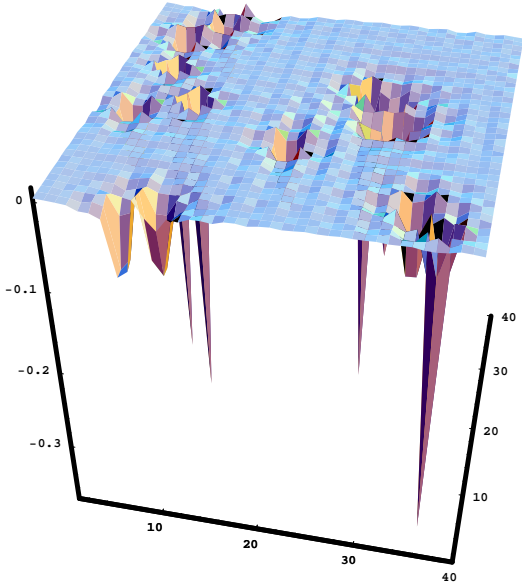


FIG. 9: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry in a disordered vortex lattice with impurities. Here $\Delta = t$, $\mu = -2.2t$, $U = 5t$, $B = 1/160$ and $n_{\text{bulk}} = 0.505$.

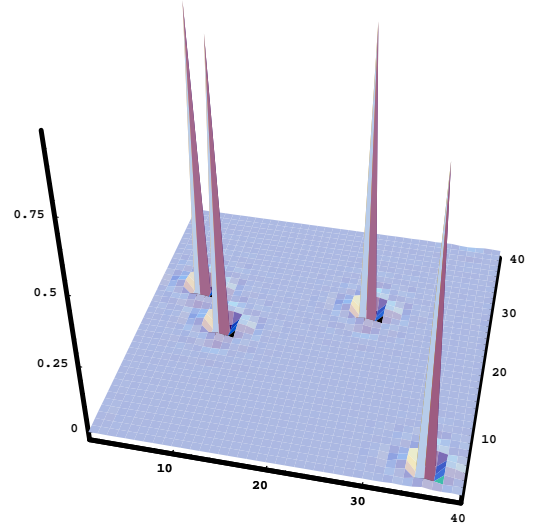


FIG. 11: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry with impurities and no vortices. Here $\Delta = t$, $\mu = -2.2t$, $U = -5t$ and $n_{\text{bulk}} = 0.513$.

the binary alloy model²⁸. At each impurity site it costs an energy U to place an electron (it acts as a local shift on the chemical potential). The impurities are randomly distributed over a $L \times L$ periodic two-dimensional lattice and play the role of pinning centers for the vortices. In general, it is favorable that a vortex is located in the vicinity of an impurity²⁹. However, in this work we will be considering random distributions of the vortices and

impurities and study the electron density throughout the system with an arbitrary distribution of the vortices and impurities. Due to the non-homogeneous nature of the order parameter the BdG equations have to be solved self-consistently.

The effect of the impurities is the expected one. If the potential is repulsive the electron density is lowered and if the potential is attractive the electron density is

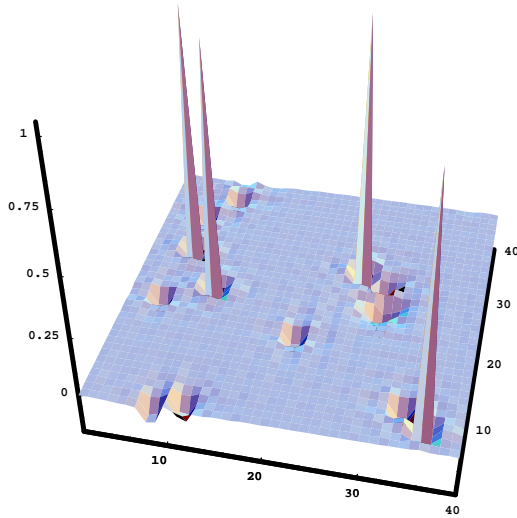


FIG. 12: (color online) Electron density $n(\mathbf{r}) - n_{\text{bulk}}$ for d-wave symmetry in a disordered vortex lattice with impurities. Here $\Delta = t$, $\mu = -2.2t$, $U = -5t$, $B = 1/160$ and $n_{\text{bulk}} = 0.509$.

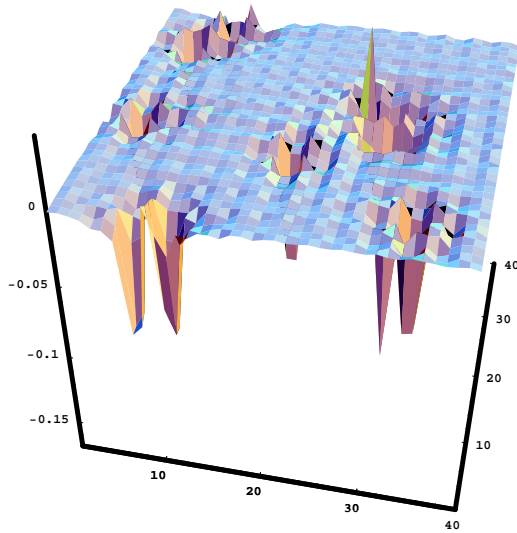


FIG. 13: (color online) Difference in the electron density between the cases with and without vortices shown in Figs. 11 and 12.

increased leading to an electron accumulation and a sign reversal. There are sharp peaks at the impurity locations that mask the effect of the vortex charge in the material. If a vortex is pinned at an impurity site (as in most systems they are) the effect of the impurity potential is quite strong. For moderate values of the potential the effect is smaller but still noticeable.

To compare the effects of the impurities and the vortices, we show in Figs. 8 and 9 the electron density for $U = 5t$ without and with vortices for a specific distribution of the impurities. In Fig. 10 we plot the difference between the two cases. We see that even though the impurities have a strong (local) influence on the charge distribution, the contributions from the impurities and the vortices add up and the difference is not negligible. The same is observed for the attractive case $U = -5t$ shown in Figs. 11, 12 and 13. Also, note that increasing the impurity potential for values $|U| > 5t$ does not change qualitatively the charge since $|U| = 5t$ is already a large value.

Clearly, when the vortices are diluted and neglecting the effect of the impurities, the interaction between the vortices is not so important and the behavior of the system is not very different from an isolated vortex. A possible exception is the regime of very high magnetic fields. But for low to intermediate fields, as seen from Figs. 1 and 2, the distortion of the electron density occurs close to the vortex locations and the behavior is characteristic of a single vortex. The vortex charge has been studied for a single vortex, as mentioned above, considering a vortex with a quantum of flux. It is therefore also interesting to consider the influence of an impurity in the single vortex case.

III. SINGLE VORTEX

We consider then the effect of an impurity in a s-wave vortex. We solve the Bogoliubov-de Gennes equations on a continuum³⁰ introducing an impurity as a disc of small radius d centered at the vortex location.

The general solution is obtained solving numerically the BdG equations. In the s-wave case these can be written as

$$\begin{aligned} (H_e + U(\mathbf{r})) u(\mathbf{r}) + \Delta(\mathbf{r}) v(\mathbf{r}) &= \epsilon u(\mathbf{r}) \\ - (H_e^* + U(\mathbf{r})) v(\mathbf{r}) + \Delta^*(\mathbf{r}) u(\mathbf{r}) &= \epsilon v(\mathbf{r}) \end{aligned} \quad (14)$$

Here

$$H_e(\mathbf{r}) = \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 + U(\mathbf{r}) - E_F$$

where m is the electron mass, \mathbf{A} is the vector potential, E_F the Fermi energy and $U(\mathbf{r})$ is the potential originated from the impurity.

The BdG equations are solved using the decompositions³⁰:

$$\begin{aligned} u^i(\rho, \varphi) &= \sum_{\mu, j} c_{\mu, j}^i e^{i\varphi\mu} \phi_{j, \mu}(\rho) \\ v^i(\rho, \varphi) &= \sum_{\mu, j} d_{\mu, j}^i e^{i\varphi\mu} \phi_{j, \mu}(\rho) \end{aligned} \quad (15)$$

and choosing a gauge such that $\Delta(\rho, \varphi) = \Delta(\rho) e^{-im\varphi}$. appropriate for a vortex containing m flux quanta. Here

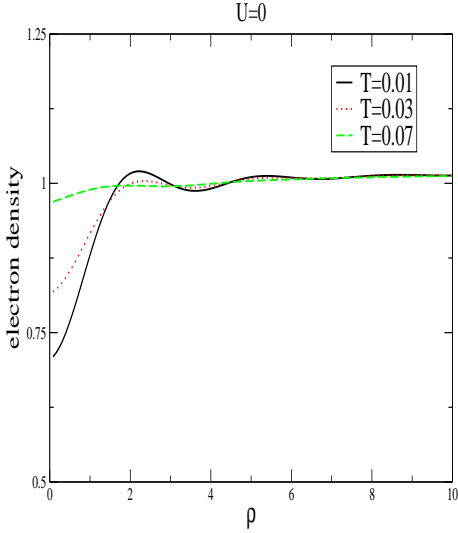


FIG. 14: (color online) Electron density of a single vortex as a function of distance for different values of T . The parameters are chosen as $E_F = 1, V = 1.6, R = 80$. The energies are in units of the Fermi energy and the lengths in units of the inverse of the Fermi momentum.

μ is an integer, j is the number of the zero of the Bessel functions in a disc of radius R and the normalized functions $\phi_{j,\mu}$ constitute a complete set over the zeros and are defined by

$$\phi_{j,\mu} = \frac{\sqrt{2}}{R J_{\mu+1}(\alpha_{j,\mu})} J_{\mu} \left(\alpha_{j,\mu} \frac{\rho}{R} \right) \quad (16)$$

Here J_{μ} is the Bessel function of order μ and $\alpha_{j,\mu}$ is the j^{th} zero of the Bessel function J_{μ} . The functions $\phi_{j,\mu}$, by construction, are zero at the border of the disc $\rho = R$. In the basis of the functions $\phi_{j,\mu}$ we have to solve a set of equations for the c and d coefficients of the form

$$\sum_{\mu',j'} \begin{pmatrix} T_{\mu,j;\mu',j'}^- & \Delta_{\mu,j;\mu',j'} \\ \Delta_{\mu,j;\mu',j'}^+ & T_{\mu,j;\mu',j'}^+ \end{pmatrix} \begin{pmatrix} c_{\mu',j'} \\ d_{\mu',j'} \end{pmatrix} = E \begin{pmatrix} c_{\mu,j} \\ d_{\mu,j} \end{pmatrix}$$

Here the various components are diagonal in the angular momentum $T_{\mu,j;\mu',j'}^{\pm} = \delta_{\mu,\mu'} T_{\mu,j;\mu',j'}^{\pm}$ and the same for the off-diagonal terms. In the case of strongly type-II superconductors and if we are interested in the low energy states, which are particularly relevant at small distances from the vortex core, the vector potential may be neglected. The various terms are then given by

$$T_{\mu,j;\mu'}^{\pm} = \mp \left(\frac{\hbar^2}{2m} \left(\frac{\alpha_{j,\mu}}{R} \right)^2 - E_F \right) \delta_{j,j'}$$

$$\mp U \int_0^d d\rho \rho \phi_{j,\mu}(\rho) \phi_{j',\mu}(\rho)$$

and

$$\Delta_{\mu,j;j'} = \int_0^R d\rho \rho \phi_{j,\mu}(\rho) \Delta(\rho) \phi_{j',\mu+m}(\rho) \quad (17)$$

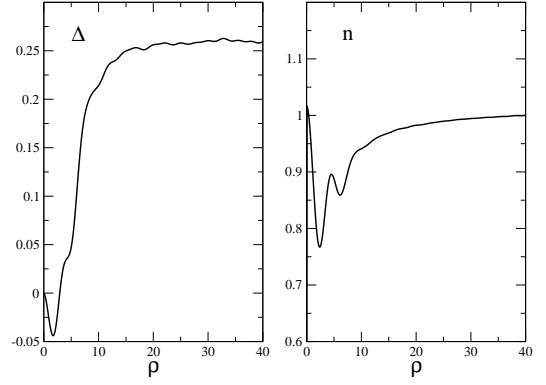


FIG. 15: Vortex with a double flux $2\Phi_0$. Left panel: Δ as a function of distance. Right panel: electron density as a function of distance

where we have used that

$$U(\rho) = U\theta(d - \rho)$$

The gap function is obtained in the usual way

$$\Delta(\rho) = V \sum_{\mu,i(|E_i| \leq \omega_D)} \bar{u}_{\mu,i}(\rho) \bar{v}_{\mu,i}(\rho) (1 - 2f(E_{\mu,i})) \quad (18)$$

with $u_{\mu,i}(\rho, \varphi) = e^{i\varphi\mu} \bar{u}_{\mu,i}(\rho)$ and $v_{\mu,i}(\rho, \varphi) = e^{i\varphi\mu+m} \bar{v}_{\mu,i}(\rho)$ where V is the attractive effective interaction between the electrons. The BdG equations are solved self-consistently, as mentioned above.

Considering first the case of a vortex enclosing a quantum of flux ($m = 1$) we show, for completeness, in Fig. 14 the charge profile close to the vortex core, considering first $U = 0$ (no impurity)⁶. Close to the vortex core the electron density decreases with respect to the bulk value. The effect is specially evident at low T . As the temperature increases the charge depletion decreases. This result is due to the Kramer and Pesch effect: the vortex core size increases as the temperature increases and, since the charge depletion may be related to the variation of the gap function³⁴, this derivative decreases as T increases and therefore the charge depletion decreases as T increases. As proposed in ref.³⁴ the electrostatic potential has contributions that are due to the difference of the gap function at the vortex with respect to the bulk value, due to the derivatives of the amplitude and of the phase of the gap function. Through Poisson's equation these dependences carry to the electron density. Note that at low T there are oscillations in the electron charge density. Also note that we are considering here the full quantum limit where we have access to the vortex structure inside the vortex core. In the previous sections the method neglected the vortex core and we had no access to the true vortex core.

As we saw in section II.B, when two vortices are close by there are also oscillations in the charge density that result, in this case, from the vicinity of two vortices. On a large scale (where the vortex core is averaged out) two

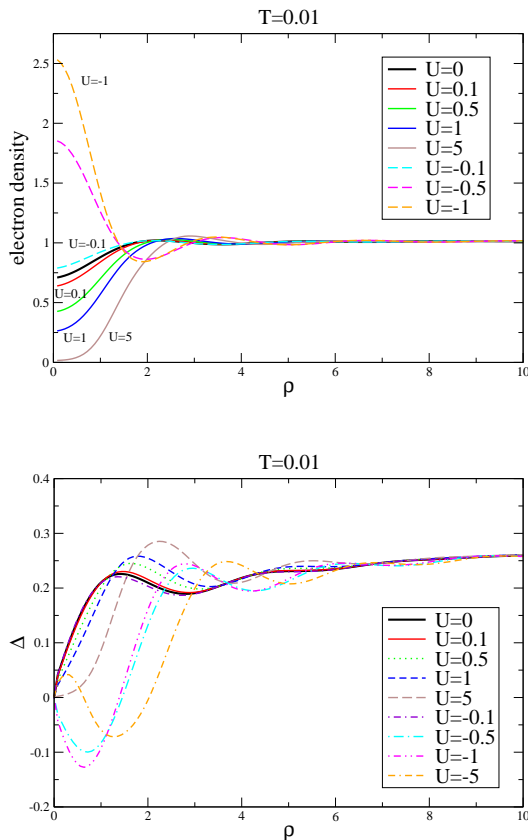


FIG. 16: (color online) Electron density and Δ as a function of distance for different values of U . The disc size is $d = 0.96$.

vortices nearby may appear similar to a vortex containing two flux quanta (note however that the energy of a double flux vortex is higher than two single quantum flux vortices). In Fig. 15 we consider the case of a vortex containing two flux quanta ($m = 2$). The inner structure of the vortex is somewhat different^{3,35}. The gap function has a node near the origin and there are opposing currents in the same regime, as also obtained using the Andreev Hamiltonian. In the right panel of Fig. 15 we show the electron density profile. As one approaches the core the charge is depleted, but very close to the location of the vortex the charge approaches the bulk value and changes sign. The trend is similar to the case studied in section II.B even though the effect is more pronounced in this last case.

In Fig. 16 we consider the effect of the impurity potential at a low value of T . For positive values of U as U increases the charge is further depleted decreasing both the value of the electron density (it vanishes at the origin for a sufficiently large value $U = 5$) and extending the regime where the charge is depleted. A value of $U = 5$ is again similar to any larger value. If the impurity potential is negative ($U < 0$) even small values of U like, for instance, $U = -0.5$ have a considerable effect on the vor-

tex charge. The attractive potential accumulates charge at the vortex core. The effect of the impurity potential on the gap function if $U > 0$ is also clear. Increasing U is similar to the effect of increasing the temperature (Kramer and Pesch effect). However, an attractive potential has a more profound effect. Even for a small value $U = -0.5$ a node appears in a way similar to the node of the vortex with two flux quanta ($m = 2$) previously considered. As U decreases further for instance for $U = -5$, two nodes appear in the gap function. Therefore, there is a similarity between the attractive impurity case, the vicinity of two vortices and the multiple-flux vortex. The quantitative effect on the vortex charge is however different, since the impurity potential is more effective in changing the signal of the vortex charge.

IV. CONCLUSIONS

Earlier treatments predicted an universal charge depletion at the vortex cores. Taking into account the competition in the d-wave case with other order parameters it has been determined that in some circumstances the vortices may be negatively charged (charge accumulation with respect to the bulk value).

In this work we did not consider the effect of other orderings but considered the influence of disorder. We focused on the effects of positional disorder of the vortices and on the effect of impurities. When two vortices are close by we found that strong fluctuations appear in the shared region of the vortices, that induce a smaller charge accumulation. Also, the addition of impurities changes the charge profiles. A small to moderate attractive potential also changes the signal of the vortex charge, since it renormalizes locally the chemical potential in a straightforward way.

The case of a vortex lattice in a very high magnetic field, where the quasiparticles propagate coherently throughout the system and gapless superconductivity occurs, is a qualitative different state. In this regime a Landau level description is adequate and a different behavior is found for many physical properties³⁶. Preliminary results seem to indicate that the effect of the coherence on the vortex charge is to change the signal of the vortex charge: close to the vortices there is a charge accumulation instead of a charge depletion³⁷. These results would then be in disagreement with possible explanations of the Hall anomaly as due to the positively charged vortices. Indeed the Hall anomaly is detected close to the normal phase, where in strongly type-II superconductors, like high- T_c materials, it is predicted that a Landau description should be appropriate¹⁷.

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- ¹ D.I. Khomskii and A. Freimuth, Phys. Rev. Lett. **75**, 1384 (1995).
 - ² F. London, *Superfluids* (Wiley, New York, 1950), Vol. I, Sec. 8.
 - ³ D. Rainer, J. A. Sauls and D. Waxman, Phys. Rev. B **54**, 10094 (1996).
 - ⁴ G. Blatter, M. Feigel'man, V. Geshkenbein, A. Larkin and A. van Otterlo, Phys. Rev. Lett. **77**, 566 (1996).
 - ⁵ K. Kumagai, K. Nozaki and Y. Matsuda, Phys. Rev. B **63**, 144502 (2001).
 - ⁶ N. Hayashi, M. Ichioka and K. Machida, J. Phys. Soc. Jpn. **67**, 3368 (1998).
 - ⁷ M. Machida and T. Koyama, Phys. Rev. Lett. **90**, 077003 (2003).
 - ⁸ J. Goryo, Phys. Rev. B **61**, 4222 (2000).
 - ⁹ J. Kolacek, P. Lipavsky and E. H. Brandt, Phys. Rev. Lett. **86**, 312 (2001).
 - ¹⁰ C. Berthod, Phys. Rev. B **71**, 134513 (2005).
 - ¹¹ M. Franz and Z. Tesařovic, Phys. Rev. Lett. **80**, 4763 (1998).
 - ¹² M. Cardoso, P. Bicudo and P.D. Sacramento, cond-mat/0509656.
 - ¹³ Y. Chen, Z.D. Wang, J.-X. Zhu and C.S. Ting, Phys. Rev. Lett. **89**, 217001 (2002).
 - ¹⁴ A.T. Dorsey et al., Phys. Rev. B **46**, 8376 (1992).
 - ¹⁵ S. Dukan and Z. Tesařovic, Phys. Rev. B **49**, 13017 (1994).
 - ¹⁶ K. Yasui and T. Kita, Phys. Rev. Lett. **83**, 4168 (1999).
 - ¹⁷ Z. Tesařovic and P.D. Sacramento, Phys. Rev. Lett. **80**, 1521 (1998).
 - ¹⁸ D.P. Arovas, A.J. Berlinsky, C. Kallin and S.-C. Zhang, Phys. Rev. Lett. **79**, 2871 (1997).
 - ¹⁹ S. Chakravarty, R. B. Laughlin, D.K. Morr and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
 - ²⁰ M. Franz, D.E. Sheehy and Z. Tesařovic, Phys. Rev. Lett. **88**, 257005 (2002).
 - ²¹ Y. Chen, Z.D. Wang and C.S. Ting, Phys. Rev. B **67**, 220501 (2003).
 - ²² M.M. Maska and M. Mierzejewski, Phys. Rev. B **68**, 024513 (2003).
 - ²³ D. Knapp, C. Kallin, A. Ghosal and S. Mansour, Phys. Rev. B **71**, 064504 (2005).
 - ²⁴ J.-X. Zhu, W. Kim, C.S. Ting and J.P. Carbotte, Phys. Rev. Lett. **87**, 197001 (2001).
 - ²⁵ A.L. Fetter and J.D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971).
 - ²⁶ M. Franz and Z. Tesařović, Phys. Rev. Lett. **84**, 554 (2000).
 - ²⁷ O. Vafek, A. Melikyan, M. Franz, and Z. Tesařović, Phys. Rev. B **63**, 134509 (2001).
 - ²⁸ W. A. Atkinson et al., Phys. Rev. Lett. **85**, 3926 (2000).
 - ²⁹ G. Blatter et al., Rev. Mod. Phys. **66**, 1125 (1994).
 - ³⁰ F. Gygi and M. Schluter, Phys. Rev. B **43**, 7609 (1991).
 - ³¹ J. Lages, P. D. Sacramento and Z. Tesařović, Phys. Rev. B **69**, 094503 (2004).
 - ³² J. Lages and P. D. Sacramento, Phys. Rev. B **71**, 132501 (2005).
 - ³³ S.H. Simon and P.A. Lee, Phys. Rev. Lett. **78**, 1548 (1997).
 - ³⁴ X.-Y. Jin and Z.-Z. Gan, Eur. Phys. Journ. B **37**, 489 (2004).
 - ³⁵ S.M.M. Virtanen and M.M. Salomaa, Phys. Rev. B **60**, 14581 (1999).
 - ³⁶ M. Rasolt and Z. Tesařovic, Rev. Mod. Phys. **64**, 709 (1992).
 - ³⁷ P. D. Sacramento, unpublished.